

Boundary Value Methods for the reconstruction of Sturm-Liouville potentials

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Abstract

In this paper we present numerical procedures for solving the two inverse Sturm-Liouville problems known in the literature as the *two-spectra* and the *half inverse* problems. The method proposed looks for a continuous approximation of the unknown potential belonging to a suitable function space of finite dimension. In order to compute such an approximation a sequence of direct problems has to be solved. This is done by applying one of the Boundary Value Methods, generalizing the classical Numerov scheme, recently introduced by the authors. Numerical results confirming the effectiveness of the approach proposed are also reported.

Key words: Boundary Value Methods, Inverse Sturm-Liouville problems, Eigenvalues.

1. Introduction

An inverse Sturm-Liouville problem (SLP) consists in reconstructing the potential function q of the differential operator

$$L = -\frac{d^2}{dx^2} + q(x)$$

from the knowledge of suitable spectral data. There exist several formulations of inverse SLPs all involving the knowledge of a complete spectrum

$$\{\lambda_k(q, a, b)\}_{k=1,2,\dots}, \quad (1)$$

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where $\lambda_k(q, a, b)$ denotes the k th eigenvalue of the direct SLP

$$Ly = -y''(x) + q(x)y(x) = \lambda y(x), \quad x \in (0, \pi), \quad (2)$$

$$\sin(a)y(0) + \cos(a)y'(0) = 0, \quad (3)$$

$$\sin(b)y(\pi) + \cos(b)y'(\pi) = 0, \quad (4)$$

with the coefficients of the boundary conditions (BCs) $a, b \in [0, \pi)$ assigned. This information, however, does not determine uniquely the potential. The additional data provided for getting the uniqueness of the solution lead to define different inverse SLPs. Among them, two problems which have received a renewed interest in the recent literature, due to their application in various branches of science, are the so-called *two-spectra* problem and the *half inverse* problem. In the first case, in addition to (1), the potential is uniquely determined by assigning a second spectrum [1]

$$\left\{ \lambda_k(q, a, \hat{b}) \right\}_{k=1,2,\dots}, \quad \hat{b} \neq b, \quad (5)$$

corresponding to a different set of boundary conditions, while in the second case the additional information is constituted by the knowledge of q over half interval of integration [2]. These are the two inverse problems we have considered in this paper.

It is known that if $q \in L^2([0, \pi])$, as we shall always assume hereafter, the k th eigenvalue $\lambda_k(q, a, b)$ behaves asymptotically as

$$\lambda_k(q, a, b) = \lambda_k(0, a, b) + \bar{q} + \delta_k(q, a, b), \quad (6)$$

where $\lambda_k(0, a, b)$ is the k th eigenvalue of the SLP with the same BCs and zero potential, $\bar{q} = \frac{1}{\pi} \int_0^\pi q(x)dx$ is the mean value of q and $\{\delta_k(q, a, b)\}_{k=1}^\infty \in \ell^2$, [3]; a more precise estimate of the remainder for smooth potential is given in [4] where it is proved that if $q \in C^2([0, \pi])$ then $\delta_k(q, a, b) = O(k^{-2})$. The consequence of (6) is that the information that the given spectrum (1) provides about the variation of the unknown potential are contained in the terms $\delta_k(q, a, b)$ and, in view of their behaviour, the first eigenvalues are the most important for the reconstruction of q . Clearly, in the case of the two-spectra inverse problem, a similar consideration can be made for the second spectrum which uniquely determines q . By virtue of this fact and of the stability analysis of inverse SLPs with finite spectral data carried out in [5],

many numerical methods currently available for the solution of inverse SLPs assume that the input data are constituted by a finite set of eigenvalues. This assumption is surely reasonable also because in the applications this is frequently the case. In the sequel, as first step in the direction of finding an approximation of the unknown potential, we will therefore assume that the first M eigenvalues of (1) are the ones effectively known and, in the case of the two-spectra problem, that this is the case also for the second spectrum.

At present time several methods have been proposed for solving inverse SLPs, [6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20]. Many of them require the solution of direct SLPs for a sequence of approximations of q . In this context, the use of matrix methods is considered appropriate. These schemes are based on the application of finite difference or finite element methods for the solution of ODEs over an assigned partition of $[0, \pi]$ frequently composed by

$$x_i = ih, \quad i = 0, 1, \dots, N+1, \quad h = \frac{\pi}{N+1}. \quad (7)$$

When applied for solving the direct SLP (2)–(4), such methods replace the continuous problem with a generalized matrix eigenvalue one of the form

$$A\mathbf{y}^{(h)} = \lambda^{(h)}S\mathbf{y}^{(h)}. \quad (8)$$

Here $\lambda^{(h)} = \lambda^{(h)}(q, a, b)$ is the approximation of one of the exact eigenvalues, $\mathbf{y}^{(h)}$ the corresponding numerical eigenfunction and the square matrices $A = A(q, a, b)$ and $S = S(q, a, b)$ depend on the particular method. As it is well-known the accuracy of the approximation $\lambda_k^{(h)}(q, a, b)$ of $\lambda_k(q, a, b)$ deteriorates significantly for increasing values of the index k so that the discretization error of a matrix method inevitably swamps the term $\delta_k(q, a, b)$ in (6) with the exception of the first few indices. The application of the asymptotic (or algebraic) correction technique, introduced in [21, 22] for the three-point formula and in [23, 24, 25] for the Numerov method, allows to greatly improve such eigenvalue estimates. It is based on the observation that the leading term in the discretization error is independent of the potential q . This has suggested to correct the estimate $\lambda_k^{(h)}(q, a, b)$ by adding to it the term

$$\epsilon_k^{(h)}(a, b) = \lambda_k(0, a, b) - \lambda_k^{(h)}(0, a, b). \quad (9)$$

Concerning the use of matrix methods for the solution of the two-spectra problem we mention the methods proposed in [6, 7]. In both papers the

methods developed are based on the application of the Numerov method for getting a pointwise approximation of q over the meshpoints of the partition (7). In particular, one of the procedures discussed in [7] computes an approximation of the potential by solving the system of $2M$ nonlinear equations, see (1)–(5) and (9),

$$\lambda_k^{(h)}(q, a, b) + \epsilon_k(a, b) - \lambda_k(q, a, b) = 0, \quad k = 1, 2, \dots, M, \quad (10)$$

$$\lambda_k^{(h)}(q, a, \hat{b}) + \epsilon_k(a, \hat{b}) - \lambda_k(q, a, \hat{b}) = 0, \quad k = 1, 2, \dots, M. \quad (11)$$

In order for the previous system of equations to be square, it is clear that the value of N in (7) has to be chosen approximately $2M$. In [6, 7], the author studied the convergence properties of the modified Newton method applied for solving (10)–(11) under the hypothesis that the unknown potential is sufficiently close to a constant function.

As further references to methods currently available for the two-spectra problem we mention the ones introduced in [9, 15] which make use of the Boundary Value Methods (BVMs) for first or second order ODEs discussed in [26, 27, 28]. In addition, in [9] the convergence properties of the Broyden method applied for solving (10)–(11) were studied.

Concerning the reconstruction of a partially known potential from the knowledge of one spectrum we cite the method proposed in [14] which uses the Numerov scheme as basic matrix method and the modified Newton method for solving (10). Another very recent contribute is due to Andrew. In [8] he discusses the possibility of recovering q also when it is known over a subinterval $[0, d]$ or $[d, \pi]$ with d not necessarily equal to $\pi/2$.

A common characteristic of all the mentioned methods is that they provide a pointwise approximation of the potential and that the number of meshpoints for the matrix methods used is constrained to be approximately $2M$. It is to be noted that frequently M is relatively small and, consequently, the accuracy of the eigenvalues estimates provided by a matrix method used over a coarse mesh may be rather poor.

Following the idea introduced by two of the authors in [29] for the symmetric inverse problem, we here propose an approach for solving the two considered inverse SLPs which overcomes such difficulty. In fact, we look for a continuous approximation of the unknown potential (eventually shifted), over the entire or half interval of integration, of the form $\sum_{i=1}^L c_i \phi_i(x)$ where $\phi_i(x)$, $i = 1, 2, \dots, L$, are linearly independent functions fixed a priori. The vector of coefficients $\mathbf{c} = (c_1, c_2, \dots, c_L)^T$ is determined by using the given spectral

data. In particular, the matrix methods introduced in [26, 27] are used for solving the sequence of direct problems involved in the iterative procedure for the computation of \mathbf{c} . The chosen value of L is constrained by the number of known eigenvalues while the value of N in (7) is left free. A system of nonlinear equations analogous to (10)-(11) in the case of the two-spectra problem or just to (10) for the problem with partially known q is formulated and solved by means of the modified Newton method. For the latter type of problem, we will consider also the possibility of getting an approximation belonging to $C^0([0, \pi])$ in the case where q is sufficiently regular in the subinterval over which it is known.

The paper is organized as follows. In Section 2 we describe the BVMs used for solving the direct SLPs involved in the procedure. In Section 3 and Section 4 we discuss the methods for the two-spectra and the half inverse problems, respectively. The results of some numerical experiments, confirming the effectiveness of the approach proposed, are then reported in Section 5.

2. The direct problem

In this section, we briefly recall the main facts concerning the BVMs introduced in [26, 27] for the approximations of the eigenvalues of the SLP (2)–(4).

These schemes are based on the application of a family of Linear Multistep Methods (LMMs) for the numerical integration of a second order ordinary differential equation of special type given by

$$y'' = f(x, y), \quad x \in [0, \pi]. \quad (12)$$

In particular, the (2ν) -step BVM ($\nu \geq 1$), applied over the uniform mesh (7), discretizes the equation as follows

$$\frac{y_{s-1} - 2y_s + y_{s+1}}{h^2} = \sum_{i=0}^{2\nu} \beta_i^{(s)} f_i, \quad s = 1, 2, \dots, \nu - 1, \quad (13)$$

$$\frac{y_{n-1} - 2y_n + y_{n+1}}{h^2} = \sum_{i=0}^{2\nu} \beta_i^{(\nu)} f_{n+i-\nu}, \quad n = \nu, \dots, N + 1 - \nu, \quad (14)$$

$$\frac{y_{m-1} - 2y_m + y_{m+1}}{h^2} = \sum_{i=0}^{2\nu} \beta_i^{(s)} f_{m-s+i}, \quad s = \nu + 1, \dots, 2\nu - 1, \quad (15)$$

$$m = N + 1 + s - 2\nu,$$

where $y_i \approx y(x_i)$ and $f_i = f(x_i, y_i)$. The coefficients $\beta_i^{(s)}$, $s = 1, 2, \dots, 2\nu - 1$, are determined by imposing all the formulae to have order of accuracy (at least) $2\nu + 1$. In particular, the formula in (14) (called *main method* [30]) turns out to be a symmetric LMM of order $p = 2\nu + 2$.

Concerning the discretization of $y'(0)$, required if $\cos(a) \neq 0$ in (3), we use the $(2\nu + 2)$ -step Forward Differentiation Formula of order $2\nu + 2$ [27]

$$\sum_{j=0}^{2\nu+2} \alpha_j y_j \approx h y'(0),$$

from which we get the following approximation of (3)

$$y_0 = \gamma_L(a) \boldsymbol{\alpha}^T \mathbf{y}^{(h)}, \quad \gamma_L(a) = -\frac{\cos(a)}{h \sin(a) + \cos(a) \alpha_0}, \quad (16)$$

where $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_{2\nu+2}, 0, \dots, 0)^T \in \mathbb{R}^N$, and $\mathbf{y}^{(h)} = (y_1, \dots, y_N)^T$. Similarly, an approximation of $y'(\pi)$ is obtained by using the $(2\nu + 2)$ -step Backward Differentiation Formula whose coefficients are $\hat{\alpha}_i = -\alpha_{2\nu+2-i}$, $i = 0, 1, \dots, 2\nu + 2$. This leads to the following discretization of (4)

$$y_{N+1} = -\gamma_R(b) \boldsymbol{\alpha}^T \hat{J} \mathbf{y}^{(h)}, \quad \gamma_R(b) = -\frac{\cos(b)}{h \sin(b) - \cos(b) \alpha_0}, \quad (17)$$

being \hat{J} the anti-identity matrix of size N .

After some computation, from (13)–(15) applied to (12) with $f(x, y) = q(x)y(x) - \lambda y(x)$ (see (2)) and (16)–(17), one obtains that the coefficient matrices $A = A(q, a, b)$ and $S = S(a, b)$ of the generalized eigenvalue problem (8) provided by the considered BVM are given by

$$\begin{aligned} A(q, a, b) = & -\frac{1}{h^2} T + B^{(\nu)} Q + \gamma_L(a) \left(-\frac{1}{h^2} \mathbf{e}_1^{(N)} + q_0 \boldsymbol{\beta}_0^{(\nu)} \right) \boldsymbol{\alpha}^T \\ & - \gamma_R(b) \hat{J} \left(-\frac{1}{h^2} \mathbf{e}_1^{(N)} + q_{N+1} \boldsymbol{\beta}_0^{(\nu)} \right) \boldsymbol{\alpha}^T \hat{J}, \end{aligned} \quad (18)$$

$$S(a, b) = B^{(\nu)} + \gamma_L(a) \boldsymbol{\beta}_0^{(\nu)} \boldsymbol{\alpha}^T - \gamma_R(b) \hat{J} \boldsymbol{\beta}_0^{(\nu)} \boldsymbol{\alpha}^T \hat{J} \quad (19)$$

where T , $B^{(\nu)}$, $\mathbf{e}_1^{(N)}$, and $\boldsymbol{\beta}_0^{(\nu)}$ are defined as in [29, Section 2], $q_i = q(x_i)$ for each i , and $Q = \text{diag}(q_1, \dots, q_N)$.

Concerning the accuracy of the so-obtained approximation of the k th eigenvalue, in [26, 27] it has been proved that if kh is “sufficiently” small and $\nu > 1$ then

$$|\lambda_k(q, a, b) - \lambda_k^{(h)}(q, a, b)| \sim O\left(k^{p+1}h^{p-\frac{1}{2}}\right) + O\left(k^{p+2}h^p\right), \quad p = 2\nu + 2.$$

In addition, there is numerical evidence that the asymptotic correction is successful in improving the eigenvalue approximations provided by the proposed BVMs.

Remark 1. *A drawback of the proposed schemes is constituted by the fact that when the order p of the method increases the spectrum of the matrix pencil (A, S) may contain some few couples of complex conjugate eigenvalues. This is in contrast with the peculiarity of a regular SLP with a real-valued potential q of having a real spectrum. A possible strategy for overcoming such incongruity consists in taking a finer mesh near the extremes of the interval of integration (see [29, Remark 2] for further details).*

3. Reconstruction of the potential from two spectra

In some cases, the two-spectra inverse SLP can be reformulated as a symmetric inverse one. This happens, for example, if the first spectrum (1) corresponds to the SLP with Dirichlet-Dirichlet BCs (i.e. $a = b = \pi/2$, see (3)-(4)) and the second spectrum (5) to the SLP with Dirichlet-Neumann BCs (i.e. $a = \pi/2$ and $\hat{b} = 0$). In the sequel, we will refer to this problem as the DD-DN inverse problem. It is known that the sequence

$$\lambda_1(q, \pi/2, 0) < \lambda_1(q, \pi/2, \pi/2) < \lambda_2(q, \pi/2, 0) < \lambda_2(q, \pi/2, \pi/2) < \dots$$

is the spectrum of the SLP

$$\begin{aligned} -z'' + \hat{q}(x)z &= \lambda z, \quad x \in (0, 2\pi), \\ z(0) &= z(2\pi) = 0, \end{aligned} \tag{20}$$

where the potential \hat{q} is obtained by extending symmetrically q , i.e.

$$\hat{q}(x) = \hat{q}(2\pi - x) = q(x), \quad \text{for } x \in [0, \pi]. \tag{21}$$

By virtue of this fact, an approximation of \hat{q} and, therefore, of q , can be computed by applying the procedure developed in [29], re-adapted appropriately

for a problem defined over $[0, 2\pi]$. The resulting method is the analogous of the method of symmetric extension proposed in [7]. A similar consideration applies also if $a = b = 0$ and $\hat{b} = \pi/2$ (NN-ND inverse problem) since $\lambda_1(q, 0, 0) < \lambda_1(q, 0, \pi/2) < \lambda_2(q, 0, 0) < \lambda_2(q, 0, \pi/2) < \dots$ is the spectrum of (20) subject to

$$z'(0) = z'(2\pi) = 0.$$

It is to be noted that, in general, the symmetric potential \hat{q} is only continuous at $x = \pi$ and, consequently, the method described in [29] provides inevitably a rather poor accurate approximation of \hat{q} in proximity of π . This consideration leads us to develop a method for solving the two-spectra inverse problem in its original formulation. If M is the number of eigenvalues of each spectrum effectively known, then the first step of this method consists in the selection of a function space $\Phi \subset L^2([0, \pi])$ of size $2M$, containing the constant functions, and of a corresponding basis

$$\mathcal{B} = \{\phi_1(x), \phi_2(x), \dots, \phi_{2M}(x)\} . \quad (22)$$

We then look for an approximation of q of the form

$$\phi(x, \mathbf{c}) = \sum_{j=1}^{2M} c_j \phi_j(x), \quad \mathbf{c} = (c_1, \dots, c_{2M})^T \in \mathbb{R}^{2M}, \quad (23)$$

where the coefficient vector \mathbf{c} is computed by using the given spectral data. Before describing how this is done, we need to introduce some notations. For any function $\psi \in L^2([0, \pi])$ let

$$\Lambda(\psi, a, b) = (\lambda_1(\psi, a, b), \dots, \lambda_M(\psi, a, b))^T \quad (24)$$

be the vector containing the first M exact eigenvalues of the SLP (2)–(4) with $q(x)$ replaced by $\psi(x)$,

$$\Lambda^{(h)}(\psi, a, b) = \left(\lambda_1^{(h)}(\psi, a, b), \dots, \lambda_M^{(h)}(\psi, a, b) \right)^T \quad (25)$$

be the vector whose entries are the corresponding numerical eigenvalues provided by the (2ν) -step BVM, ν a priori fixed, used with stepsize h , and let

$$E^{(h)}(a, b) = \left(\epsilon_1^{(h)}(a, b), \dots, \epsilon_M^{(h)}(a, b) \right)^T, \quad (26)$$

where $\epsilon_k^{(h)}(a, b)$ is the asymptotic correction term for the k th eigenvalue given in (9).

The vectors $\Lambda(\psi, a, \hat{b})$, $\Lambda^{(h)}(\psi, a, \hat{b})$ and $E^{(h)}(a, \hat{b})$ are defined similarly for the second spectrum (5). Finally, let

$$\Lambda(\psi) = \begin{pmatrix} \Lambda(\psi, a, b) \\ \Lambda(\psi, a, \hat{b}) \end{pmatrix}, \quad \Lambda^{(h)}(\psi) = \begin{pmatrix} \Lambda^{(h)}(\psi, a, b) \\ \Lambda^{(h)}(\psi, a, \hat{b}) \end{pmatrix}, \quad (27)$$

$$E^{(h)} = \begin{pmatrix} E^{(h)}(a, b) \\ E^{(h)}(a, \hat{b}) \end{pmatrix}. \quad (28)$$

With this notation, the vector $\Lambda(q)$ contains the input data of the two-spectra problem. The coefficient vector \mathbf{c} , which determines the approximation $\phi(x, \mathbf{c}) \approx q(x)$, see (23), is then computed by solving the following system of $2M$ nonlinear equations

$$F^{(h)}(\mathbf{c}) = \Lambda^{(h)}(\phi(\cdot, \mathbf{c})) + E^{(h)} - \Lambda(q) = \mathbf{0}, \quad (29)$$

where $\mathbf{0}$ is the zero vector in \mathbb{R}^{2M} . This means that we look for a function $\phi(\cdot, \mathbf{c}) \in \Phi$ for which the corresponding first M corrected numerical eigenvalues of both SLPs, provided by the selected BVM, coincide with the exact ones given for the unknown potential. As mentioned in the introduction, it must be underlined the fact that, with this approach, the choice of the stepsize h is independent of the number of known eigenvalue. This implies that, in exact arithmetic, the error in the approximation $\Lambda^{(h)}(\phi(\cdot, \mathbf{c})) + E^{(h)} \approx \Lambda(\phi(\cdot, \mathbf{c}))$ can be considered as a small perturbation for h sufficiently small. In particular, if $q \in \Phi$ the flexibility in the choice of the stepsize allows to reconstruct it with arbitrarily high accuracy.

Concerning the solution of the system of nonlinear equations (29), it is clear that the classical Newton method may be used. Nevertheless, the application of Newton-like methods is frequently preferred due to their lower computational cost per iteration. For example, in [9] the application of the Broyden method has been considered while in [7, 10] the modified Newton method has been used. The latter one has satisfactory convergence properties in the case where the unknown potential is “sufficiently” close to a constant function. This is the method we have used in this paper. The corresponding recurrence relation is given by

$$\mathbf{c}_{r+1}^{(h)} = \mathbf{c}_r^{(h)} - (J^{(h)}(\mathbf{0}))^{-1} F^{(h)}(\mathbf{c}_r^{(h)}), \quad r = 0, 1, 2, \dots, \quad (30)$$

where $\mathbf{c}_0^{(h)}$ is an assigned initial approximation and $J^{(h)}(\mathbf{0})$ is the Jacobian matrix

$$J^{(h)}(\mathbf{c}) = \frac{\partial F^{(h)}(\mathbf{c})}{\partial \mathbf{c}} = \frac{\partial \Lambda^{(h)}(\phi(\cdot, \mathbf{c}))}{\partial \mathbf{c}},$$

evaluated at $\mathbf{c} = \mathbf{0}$. From (25)–(28), one immediately gets

$$(J^{(h)}(\mathbf{c}))_{kj} = \frac{\partial \lambda_k^{(h)}(\phi(\cdot, \mathbf{c}), a, b)}{\partial c_j}, \quad (J^{(h)}(\mathbf{c}))_{k+M,j} = \frac{\partial \lambda_k^{(h)}(\phi(\cdot, \mathbf{c}), a, \hat{b})}{\partial c_j},$$

for each $k = 1, 2, \dots, M$ and $j = 1, 2, \dots, 2M$. The formula for the computation of the previous partial derivatives is similar to the one given in [29] and we don't report it here. As done in the paper just cited, we assume hereafter that

$$\lim_{h \rightarrow 0} J^{(h)}(\mathbf{0}) = \lim_{h \rightarrow 0} \left. \frac{\partial \Lambda^{(h)}(\phi(\cdot, \mathbf{c}))}{\partial \mathbf{c}} \right|_{\mathbf{c}=\mathbf{0}} = \left. \frac{\partial \Lambda(\phi(\cdot, \mathbf{c}))}{\partial \mathbf{c}} \right|_{\mathbf{c}=\mathbf{0}} \equiv J(\mathbf{0}), \quad (31)$$

whose entries are known to be given by [18]

$$(J(\mathbf{0}))_{kj} = \frac{\int_0^\pi y_k^2(x) \phi_j(x) dx}{\int_0^\pi y_k^2(x) dx}, \quad (J(\mathbf{0}))_{k+M,j} = \frac{\int_0^\pi \hat{y}_k^2(x) \phi_j(x) dx}{\int_0^\pi \hat{y}_k^2(x) dx}, \quad (32)$$

for each $k = 1, 2, \dots, M$ and $j = 1, 2, \dots, 2M$. In the previous formula, $y_k(x)$ and $\hat{y}_k(x)$ are the k th exact eigenfunction for the SLP with zero potential and BCs determined by a and b or a and \hat{b} , respectively.

It is important to remark that the criterion we have used for the choice of the function space Φ has been that of finding a good compromise between the accuracy of the best approximation, in L^2 -norm, of q that we can find inside of it and the stability properties of the resulting procedure for the solution of the inverse problem. In [29], this compromise has been obtained with the space of symmetric trigonometric polynomials and the space of symmetric cubic spline functions. We have therefore considered analogous function spaces for solving the two-spectra inverse problem.

3.1. Trigonometric polynomials

In the context of trigonometric polynomials it seems natural to consider the function space spanned by the following basis functions

$$\phi_{2j-1}(x) = \cos(2(j-1)x), \quad \phi_{2j}(x) = \sin(2jx), \quad j = 1, 2, \dots, M.$$

The corresponding best approximation, in L^2 -norm, of the potential, given by

$$\phi(x, \mathbf{c}^*) = \sum_{j=1}^{2M} c_j^* \phi_j(x), \quad c_j^* = \frac{\int_0^\pi q(x) \phi_j(x) dx}{\int_0^\pi \phi_j^2(x) dx}, \quad (33)$$

is the truncated Fourier series of the periodic extension of q with period π . It is known, however, that if q is sufficiently regular, as we always assume hereafter, then the error with respect to such best approximation decreases as $O(M^{-1/2})$. We therefore prefer to consider the space Φ with coordinate functions given by

$$\phi_j(x) = \cos((j-1)x), \quad j = 1, 2, \dots, 2M. \quad (34)$$

With this choice, in fact, the best approximation (33) is the truncated Fourier series of the periodic extension with period 2π of the symmetric function \hat{q} in (21). It follows that $\|q - \phi(\cdot, \mathbf{c}^*)\| = O(M^{-3/2})$.

For the analysis of the stability properties of the resulting procedure, we take as a model the conditioning of the limit Jacobian (31)-(32) associated to (34). This can be studied analytically in the case of the DD-DN or the NN-ND two-spectra inverse problems since $J(\mathbf{0})$ turns out to have a simple structure. In more details, let's consider the DD-DN problem. The k th eigenfunction of (2)-(4) with $q(x) \equiv 0$ and BCs $y(0) = y(\pi) = 0$ or $y(0) = y'(\pi) = 0$ is $y_k(x) = \sin(kx)$ or $y_k(x) = \sin((k-0.5)x)$, respectively. From (32) after some computations one verifies that $J(\mathbf{0})$ is a scaled Frobenius matrix with permuted rows. More precisely, the only nonzero entries of $J(\mathbf{0})$ for the DD-DN problem are given by

$$\begin{aligned} (J(\mathbf{0}))_{k1} &= 1, \quad k = 1, 2, \dots, 2M, \\ (J(\mathbf{0}))_{k, 2k+1} &= -0.5, \quad k = 1, 2, \dots, M-1, \\ (J(\mathbf{0}))_{k+M, 2k} &= -0.5, \quad k = 1, 2, \dots, M. \end{aligned}$$

For the NN-ND inverse problem, it results that the only nonzero entries of $J(\mathbf{0})$ are given by

$$\begin{aligned} (J(\mathbf{0}))_{k1} &= 1, \quad k = 1, 2, \dots, 2M, \\ (J(\mathbf{0}))_{k, 2k-1} &= 0.5, \quad k = 2, 3, \dots, M, \\ (J(\mathbf{0}))_{k+M, 2k} &= 0.5, \quad k = 1, 2, \dots, M. \end{aligned}$$

since the k th eigenfunction of (2)–(4) with $q(x) \equiv 0$ and BCs $y'(0) = y'(\pi) = 0$ or $y'(0) = y(\pi) = 0$ is $y_k(x) = \cos((k-1)x)$ or $y_k(x) = \cos((k-0.5)x)$, respectively. We observe that $J(\mathbf{0})$ is a lower triangular matrix with permuted rows.

In both the previous cases, the spectral condition number of $J(\mathbf{0})$, which can be computed analytically, grows linearly with respect to M .

3.2. Cubic spline functions

The other space of functions we have considered is the space of cubic spline functions. In this case, the conditioning of the limit Jacobian (31) and, consequently, the stability of the procedure depends strictly on the choice of the partition of $[0, \pi]$. The partitions that we have used are of the following type

$$\Delta : t_0 = 0 < t_1 < \dots < t_{2M-3} = \pi, \quad (35)$$

$$t_1 = \omega_1 h_t, \quad t_i = t_{i-1} + h_t, \quad i = 2, \dots, 2M-4, \quad t_{2M-3} = t_{2M-4} + \omega_2 h_t, \quad (36)$$

where ω_1 and ω_2 are suitable positive constants and $h_t = \pi/(2M + \omega_1 + \omega_2 - 5)$. The basis (22) used is constituted by the B-spline functions of order four, normalized to have L^2 -norm equal to one, relative to the knot sequence $\{t_i\}_{i=-3}^{2M}$, with $t_{-i} = -ih_t$ and $t_{2M-3+i} = \pi + ih_t$ for $i = 1, 2, 3$.

Remark 2. *The most natural choice would be the use of a uniform partition for $[0, \pi]$ which corresponds to $\omega_1 = \omega_2 = 1$. Unfortunately, the stability properties of the resulting method turn out to be definitely unsatisfactory. This is caused by the fact that the support of the first and the last basis functions is too small. In order to improve the stability of the method, we therefore use a partition with the first and the last subintervals larger than the others, namely ω_1 and ω_2 are chosen larger than one.*

In Table 1, the asymptotic behaviours of $\kappa(J(\mathbf{0}))$, the conditioning in euclidean norm of the limit Jacobian (31), have been reported for the DD-DN and the NN-ND problems and some values of (ω_1, ω_2) . It is evident that $(\omega_1, \omega_2) = (1, 1)$ (uniform mesh) is a bad choice, as said before. Instead, the best choice for the former problem is $(\omega_1, \omega_2) = (3, 2)$; the behaviour of $\kappa(J(\mathbf{0}))$ coincides with that observed in [29] for the limit Jacobian associated

to the symmetric problem with Dirichlet BCs at both ends. Similar considerations apply to the NN-ND problem with $(\omega_1, \omega_2) = (2, 2)$ when compared with the symmetric case subject to Neumann BCs at both ends.

Table 1: Conditioning of the limit Jacobian $J(\mathbf{0})$ for the spline function spaces for some partitions (35)-(36).

M	$(\omega_1, \omega_2) = (1, 1)$		$(\omega_1, \omega_2) = (2, 2)$		$(\omega_1, \omega_2) = (3, 2)$	
	$\kappa(J(\mathbf{0}))$	Rate	$\kappa(J(\mathbf{0}))$	Rate	$\kappa(J(\mathbf{0}))$	Rate
DD-DN boundary conditions						
10	$9.05e + 03$	—	$5.37e + 02$	—	$9.91e + 01$	—
20	$1.78e + 05$	—	$2.06e + 03$	—	$1.45e + 02$	—
40	$3.20e + 06$	4.16	$8.17e + 03$	2.01	$2.08e + 02$	0.47
80	$5.46e + 07$	4.09	$3.28e + 04$	2.01	$2.96e + 02$	0.49
160	$9.01e + 08$	4.04	$1.31e + 05$	2.00	$4.20e + 02$	0.49
NN-ND boundary conditions						
10	$2.62e + 02$	—	$1.03e + 02$	—	$1.45e + 02$	—
20	$1.09e + 03$	—	$1.92e + 02$	—	$3.11e + 02$	—
40	$4.54e + 03$	2.05	$3.70e + 02$	0.99	$7.25e + 02$	1.32
80	$1.86e + 04$	2.02	$2.62e + 02$	1.00	$1.81e + 03$	1.38
160	$7.51e + 04$	2.01	$1.43e + 03$	1.00	$4.72e + 03$	1.43

4. Reconstruction of a partially known potential

The further inverse problem we have tackled in this paper is the half inverse problem characterized by the knowledge of the potential over half interval of integration which, without loss of generality, we assume hereafter to be $[0, \pi/2]$. The knowledge of the spectrum of one corresponding SLP uniquely determines the values of q on the other half of the interval. In order to compute an approximation of such values, we assume that the first M eigenvalues of the spectrum are given.

An approach analogous to the one considered in the previous section can be used for the reconstruction of the unknown part of the potential. In particular, we look for a vector $\mathbf{c} = (c_1, \dots, c_M)^T \in \mathbb{R}^M$ so that

$$q(x) \approx \phi_0(x) + \sum_{j=1}^M c_j \phi_j(x) \equiv \phi_0(x) + \psi(x, \mathbf{c}), \quad x \in (\pi/2, \pi], \quad (37)$$

where $\phi_j \in L^2([\pi/2, \pi])$, $j = 0, 1, \dots, M$, are sufficiently regular functions fixed a priori with ϕ_j , $j = 1, 2, \dots, M$, linearly independent. For any $\mathbf{c} \in \mathbb{R}^M$, we denote with

$$\phi(x, q, \mathbf{c}) = \begin{cases} q(x) & \text{for } x \in [0, \pi/2], \\ \phi_0(x) + \psi(x, \mathbf{c}) & \text{for } x \in (\pi/2, \pi]. \end{cases} \quad (38)$$

The coefficient vector \mathbf{c} is computed by solving the following system of M nonlinear equations

$$F^{(h)}(\mathbf{c}) = \Lambda^{(h)}(\phi(\cdot, q, \mathbf{c})) + E^{(h)} - \Lambda(q) = \mathbf{0}. \quad (39)$$

In the previous equation, see (24)–(26), $E^{(h)} = E^{(h)}(a, b)$, and

$$\Lambda(q) = \Lambda(q, a, b), \quad \Lambda^{(h)}(\phi(\cdot, q, \mathbf{c})) = \Lambda^{(h)}(\phi(\cdot, q, \mathbf{c}), a, b),$$

where a and b are the coefficients of the BCs of the SLP of the assigned spectrum. The following two versions of the procedure have been considered:

V₁: $\phi_0(x) \equiv 0$ and the remaining ϕ_j such that $\text{span}\{\phi_1, \phi_2, \dots, \phi_M\}$ contains the constant functions;

V₂: $\phi_0(x) \equiv q(\pi/2)$ and $\phi_j(x)$ such that $\phi_j(\pi/2) = 0$ for each $j = 1, 2, \dots, M$.

Clearly, in the former case, in general, the resulting function $\phi(x, q, \mathbf{c})$ is not continuous at the matching point $x = \pi/2$. In the latter case, instead, $\phi(x, q, \mathbf{c})$ is surely continuous at such point and this may be a reasonable constraint if q is sufficiently regular over the first half of the interval of integration.

If the unknown potential is sufficiently close to a constant function then the modified Newton method can be applied for solving (39). The corresponding iteration is given by

$$\mathbf{c}_{r+1}^{(h)} = \mathbf{c}_r^{(h)} - (J^{(h)}(q, \mathbf{c}_0))^{-1} F^{(h)}(\mathbf{c}_r^{(h)}), \quad r = 0, 1, 2, \dots, \quad (40)$$

where, see (37)-(38), $\mathbf{c}_0^{(h)} \equiv \mathbf{c}_0 = (c_{1,0}, c_{2,0}, \dots, c_{M,0})^T$ is such that

$$\phi_0(x) + \sum_{j=1}^M c_{j,0} \phi_j(x) = q(\pi/2), \quad \forall x \in (\pi/2, \pi],$$

and $J^{(h)}(q, \mathbf{c}_0)$ is the Jacobian matrix

$$J^{(h)}(q, \mathbf{c}) = \frac{\partial F^{(h)}(\mathbf{c})}{\partial \mathbf{c}} = \frac{\partial \Lambda^{(h)}(\phi(\cdot, q, \mathbf{c}))}{\partial \mathbf{c}} \quad (41)$$

evaluated at $\mathbf{c} = \mathbf{c}_0$. The entries of the previous matrix depends on the BVM used. Let us assume, for simplicity, that such method is applied over a mesh (7) with $N = 2K$, $K \in \mathbb{N}$. The coefficient matrix (18) of the generalized eigenvalue problem provided by the (2ν) -step BVM applied to the SLP (2)–(4) with potential $\phi(x, q, \mathbf{c})$ can be decomposed as

$$A(\phi(\cdot, q, \mathbf{c})) \equiv A(\phi(\cdot, q, \mathbf{c}), a, b) = A_0(q) + \sum_{j=1}^M c_j A_j,$$

where, by denoting with

$$\begin{aligned} Q_0(x) &= \text{diag}(q(x_1), \dots, q(x_K), \phi_0(x_{K+1}), \dots, \phi_0(x_{2K})), \\ Q_j(x) &= \text{diag}(0, \dots, 0, \phi_j(x_{K+1}), \dots, \phi_j(x_{2K})), \quad j = 1, 2, \dots, M, \end{aligned}$$

and by letting $\gamma_L \equiv \gamma_L(a)$ and $\gamma_R \equiv \gamma_R(b)$, see (16)-(17),

$$A_0(q) = -\frac{1}{h^2}T + B^{(\nu)}Q_0 + \gamma_L \left(-\frac{1}{h^2}\mathbf{e}_1^{(N)} + q(0)\boldsymbol{\beta}_0^{(\nu)} \right) \boldsymbol{\alpha}^T + \gamma_R \hat{J} \frac{1}{h^2}\mathbf{e}_1^{(N)} \boldsymbol{\alpha}^T \hat{J}$$

$$A_j = B^{(\nu)}Q_j - \gamma_R \phi_j(x_{N+1}) \hat{J} \boldsymbol{\beta}_0^{(\nu)} \boldsymbol{\alpha}^T \hat{J}.$$

It follows that the entries of the Jacobian matrix are given by

$$(J^{(h)}(q, \mathbf{c}))_{kj} = \frac{\left\langle \mathbf{v}_k^{(h)}(q, \mathbf{c}), S^{-1} A_j \mathbf{y}_k^{(h)}(q, \mathbf{c}) \right\rangle}{\left\langle \mathbf{v}_k^{(h)}(q, \mathbf{c}), \mathbf{y}_k^{(h)}(q, \mathbf{c}) \right\rangle}$$

where $S = S(a, b)$ is defined in (19) and assumed to be nonsingular, $\langle \cdot, \cdot \rangle$ is the usual scalar product in \mathbb{R}^N and $\mathbf{v}_k^{(h)}(q, \mathbf{c})$ and $\mathbf{y}_k^{(h)}(q, \mathbf{c})$ are the k th right

and left eigenvectors of $S^{-1}A(\phi(\cdot, q, \mathbf{c}))$, respectively.

In the sequel, we shall assume that if q is sufficiently close to a constant then, see (41),

$$\lim_{h \rightarrow 0} J^{(h)}(q, \mathbf{c}_0) = \frac{\partial \Lambda(\phi(\cdot, q, \mathbf{c}_0))}{\partial \mathbf{c}} \equiv J(q, \mathbf{c}_0). \quad (42)$$

Its entries are given by [18]

$$(J(q, \mathbf{c}_0))_{kj} = \frac{\int_{\pi/2}^{\pi} y_k^2(x) \phi_j(x) dx}{\int_0^{\pi} y_k^2(x) dx}, \quad (43)$$

where $y_k(x)$ is the k th exact eigenfunction for the SLP with potential $\phi(\cdot, q, \mathbf{c}_0)$ and BCs determined by a and b , respectively.

In the following subsections, we describe the function spaces we have considered for the two versions \mathbf{V}_1 and \mathbf{V}_2 of the procedure.

4.1. Trigonometric polynomials

In the case of version \mathbf{V}_1 the basis functions we have considered are

$$\phi_j(x) = \cos(2(j-1)x), \quad j = 1, 2, \dots, M,$$

which are orthogonal over $[\pi/2, \pi]$. We recall that for this version $\phi_0(x)$ is identically zero. The corresponding best approximation, in L^2 -norm, of q over $(\pi/2, \pi]$ is therefore given by, see (37),

$$\psi(x, \mathbf{c}^*) = \sum_{j=1}^M c_j^* \phi_j(x), \quad c_j^* = \frac{\int_{\pi/2}^{\pi} q(x) \phi_j(x) dx}{\int_{\pi/2}^{\pi} \phi_j^2(x) dx}.$$

If we let

$$\tilde{q}(x) = \begin{cases} q(\pi - x) & x \in [0, \pi/2] \\ q(x) & x \in (\pi/2, \pi] \\ q(2\pi - x) & x \in (\pi, 3\pi/2] \\ q(x - \pi) & x \in (3\pi/2, 2\pi] \end{cases}$$

then one can verify that

$$c_j^* = \frac{\int_{\pi/2}^{\pi} q(x) \phi_j(x) dx}{\int_{\pi/2}^{\pi} \phi_j^2(x) dx} = \frac{\int_0^{2\pi} \tilde{q}(x) \phi_j(x) dx}{\int_0^{2\pi} \phi_j^2(x) dx}.$$

In addition, one gets

$$\int_0^{2\pi} \tilde{q}(x) \sin(jx) dx = \int_0^{2\pi} \tilde{q}(x) \cos((2j-1)x) dx = 0, \quad j = 1, 2, \dots$$

This implies that $\psi(\cdot, \mathbf{c}^*)$ is the truncated Fourier series of the periodic extension of \tilde{q} with period 2π . In a way analogous to the trigonometric polynomials used for the two-spectra inverse problem, we deduce that the error with respect to the best approximation in $[\pi/2, \pi]$ decreases as $O(M^{-3/2})$ provided q is sufficiently regular.

For the analysis of the stability properties of the resulting procedure we take as a model the conditioning of the limit Jacobian $J(0, \mathbf{0})$ (see (42)-(43)). This matrix clearly depends on the BCs of the assigned spectrum and its entries can be computed analytically in the case of natural ones. In particular, as one may expect, $J(0, \mathbf{0})$ is half the limit Jacobian obtained in [29, Section 3.1] for the symmetric inverse problem in the case of DD or NN BCs. This immediately implies that $\kappa(J(0, \mathbf{0}))$ grows linearly with respect to M . For the problems with nonsymmetric BCs, i.e., DN or ND BCs, the behaviour of such condition number has been derived experimentally. The obtained results are reported in Table 2.

Table 2: Conditioning of the limit Jacobian $J(0, \mathbf{0})$ for the trigonometric function space for the version \mathbf{V}_1 of the procedure.

M	DN BCs		ND BCs	
	$\kappa(J(0, \mathbf{0}))$	Rate	$\kappa(J(0, \mathbf{0}))$	Rate
10	1.97 + 01	—	1.62 + 02	—
20	3.43 + 01	—	4.55 + 02	—
40	6.33 + 01	0.99	1.28 + 03	1.49
80	1.21 + 02	0.99	3.61 + 03	1.50
160	2.36 + 02	0.99	1.02 + 04	1.50

Let us now consider the version \mathbf{V}_2 of the procedure. It is clear that in this case we look for a function $\psi(\cdot, \mathbf{c})$ in (37) which approximate the shifted

potential

$$z(x) = q(x) - q(\pi/2)$$

over $(\pi/2, \pi]$. This leads us to use the following coordinate functions

$$\phi_j(x) = \cos((2j-1)x), \quad j = 1, 2, \dots, M$$

which clearly satisfy the requirement $\phi_j(\pi/2) = 0$. The coefficients c_j^* of the corresponding best approximation of $z(x)$ verify

$$c_j^* = \frac{\int_{\pi/2}^{\pi} z(x) \phi_j(x) dx}{\int_{\pi/2}^{\pi} \phi_j^2(x) dx} = \frac{\int_0^{2\pi} \tilde{z}(x) \phi_j(x) dx}{\int_0^{2\pi} \phi_j^2(x) dx}$$

where

$$\tilde{z}(x) = \begin{cases} -z(\pi - x) & x \in [0, \pi/2] \\ z(x) & x \in (\pi/2, \pi] \\ z(2\pi - x) & x \in (\pi, 3\pi/2] \\ -z(x - \pi) & x \in (3\pi/2, 2\pi] \end{cases}.$$

We observe that $\tilde{z}(x)$ is symmetric with respect to $x = \pi$ and its restriction to $[0, \pi]$ is symmetric with respect to the point $(\pi/2, 0)$. It follows that $\psi(\cdot, \mathbf{c}^*)$ is the truncated Fourier series of the periodic extension of \tilde{z} with period 2π . Therefore, the considerations done for version \mathbf{V}_1 on the behaviour of the error of the best approximation hold in this case too.

Concerning the resulting conditioning of $J(0, \mathbf{0})$ the situation is reversed with respect to version \mathbf{V}_1 . In particular, for the two problems with symmetric BCs the numerically observed behaviours of $\kappa(J(0, \mathbf{0}))$ are reported in Table 3.

For the problems with DN or ND BCs, instead, the rate of growth of $\kappa(J(0, \mathbf{0}))$ has been determined theoretically. The k th eigenfunctions for the corresponding problems with zero potential are $y_k(x) = \sin(k - 0.5x)$ and $y_k(x) = \cos(k - 0.5x)$, respectively. From (43), after some computations, one deduces that

$$J(0, \mathbf{0}) = \frac{(-1)^\ell}{4} I + EE^T D \equiv J_\ell, \quad \text{with } \ell = \begin{cases} 1 & \text{for DN BCs} \\ 2 & \text{for ND BCs} \end{cases}, \quad (44)$$

where I is the identity matrix of size M , $E = (1, 1, \dots, 1)^T \in \mathbb{R}^M$ and D is a diagonal matrix whose nonzero entries are

$$d_j = \frac{(-1)^j}{\pi(2j-1)}, \quad j = 1, 2, \dots, M. \quad (45)$$

Table 3: Conditioning of the limit Jacobian $J(0, \mathbf{0})$ for the trigonometric function space for the version \mathbf{V}_2 of the procedure.

M	DD BCs		NN BCs	
	$\kappa(J(0, \mathbf{0}))$	Rate	$\kappa(J(0, \mathbf{0}))$	Rate
10	2.96 + 01	—	1.50 + 01	—
20	6.11 + 01	—	2.90 + 01	—
40	1.27 + 02	1.06	5.73 + 01	1.00
80	2.63 + 02	1.06	1.14 + 02	1.00
160	5.47 + 02	1.05	2.27 + 02	1.00

The decomposition in (44) allows to prove the following results.

Proposition 4.1. *The limit Jacobians J_ℓ in (44) are nonsingular for $\ell = 1, 2$.*

Proof: By the Sherman-Morrison formula it is sufficient to verify that $1 + 4(-1)^\ell \eta_M \neq 0$ where

$$\eta_M = E^T D E = \frac{1}{\pi} \sum_{j=1}^M \frac{(-1)^j}{2j-1} \quad (46)$$

but the mentioned inequality holds true trivially since η_M is irrational for each M .

Proposition 4.2. *The condition numbers in euclidean norm of the limit Jacobians J_ℓ in (44), verify*

$$\kappa(J_\ell) = O(M^\ell), \quad \ell = 1, 2. \quad (47)$$

Proof: It is known that

$$\kappa^2(J_\ell) = \frac{\max_{\xi \in \sigma(J_\ell J_\ell^T)} \xi}{\min_{\xi \in \sigma(J_\ell J_\ell^T)} \xi} \quad (48)$$

since J_ℓ is nonsingular as just proved.

We shall therefore study the spectrum of $J_\ell J_\ell^T$. If we denote with

$$\gamma_M = E^T D^2 E \quad (49)$$

then, from (44) one gets

$$\begin{aligned} J_\ell J_\ell^T &= \frac{1}{16}I + \frac{(-1)^\ell}{4} (D E E^T + E E^T D) + \gamma_M E E^T \\ &= \frac{1}{16}I + \frac{1}{4} ((-1)^\ell D + 2\gamma_M I) E E^T + \frac{1}{4} E E^T ((-1)^\ell D + 2\gamma_M I) \quad (50) \\ &= \frac{1}{16}I + \frac{1}{4}W, \end{aligned}$$

where

$$W = \mathbf{u}_\ell E^T + E \mathbf{u}_\ell^T, \quad \mathbf{u}_\ell = ((-1)^\ell D + 2\gamma_M I) E.$$

We observe that $\text{rank}(W) = 2$ since \mathbf{u}_ℓ and E are linearly independent. In addition, its nonzero eigenvalues, say $\mu_{1,2}$, are the eigenvalues of

$$V = \begin{pmatrix} \mathbf{u}_\ell^T E & \mathbf{u}_\ell^T \mathbf{u}_\ell \\ E^T E & \mathbf{u}_\ell^T E \end{pmatrix}.$$

It is possible to verify, after some computations, that the characteristic equation is

$$\mu^2 - (4M\gamma_M + 2(-1)^\ell \eta_M)\mu + \eta_M^2 - M\gamma_M = 0 \quad (51)$$

where η_M and γ_M are defined in (46) and (49), respectively. It follows that the eigenvalues of V are

$$\mu_{1,2} = 2M\gamma_M + (-1)^\ell \eta_M \mp \sqrt{(2M\gamma_M + (-1)^\ell \eta_M)^2 - \eta_M^2 + M\gamma_M} \quad (52)$$

with $\mu_1 < 0 < \mu_2$ since, see (45),

$$\begin{aligned} \mu_1 \mu_2 &= \eta_M^2 - M\gamma_M = \left(\sum_{j=1}^M d_j \right)^2 - M \sum_{j=1}^M d_j^2 \\ &= 2 \sum_{\substack{i,j=1 \\ i < j}}^M d_i d_j - (M-1) \sum_{i=1}^M d_i^2 = - \sum_{\substack{i,j=1 \\ i < j}}^M (d_i - d_j)^2 < 0. \end{aligned}$$

Therefore, from (50), one gets that the spectrum of $J_\ell J_\ell^T$ is given by

$$0 < \xi_1 = \frac{1}{16} + \frac{1}{4}\mu_1 < \xi_2 = \cdots = \xi_{M-1} = \frac{1}{16} < \xi_M = \frac{1}{16} + \frac{1}{4}\mu_2.$$

Consequently, see (48),

$$\begin{aligned} \kappa^2(J_\ell) &= \frac{\xi_M}{\xi_1} = \frac{1 + 4\mu_2}{1 + 4\mu_1} = \frac{(1 + 4\mu_2)^2}{1 + 4(\mu_1 + \mu_2) + 16\mu_1\mu_2} \\ &= \frac{(1 + 4\mu_2)^2}{1 + 4(4M\gamma_M + 2(-1)^\ell\eta_M) + 16(\eta_M^2 - M\gamma_M)} \\ &= \frac{(1 + 4\mu_2)^2}{(1 + 4(-1)^\ell\eta_M)^2} \end{aligned}$$

where in the second last equality we have used the fact that μ_1 and μ_2 are the roots of (51). We observe that $\gamma_M = O(1)$, see (49), and by using the Leibniz formula $\eta_M = -\frac{1}{4} + O(\frac{1}{M})$, see (46).

These equalities imply that $1 + 4\mu_2 = O(M)$, see (52), and $1 + 4(-1)^\ell\eta_M = O(M^{1-\ell})$ so that (47) is proved.

4.2. Cubic spline functions

The approach used for the space of cubic spline functions is rather similar to the one considered in Section 3.2. In particular, the structure of the partitions of $[\pi/2, \pi]$ used is the following

$$\Delta : t_0 = \frac{\pi}{2} < t_1 < \cdots < t_{L-3} = \pi, \quad (53)$$

$$t_1 = t_0 + \omega_1 h_t, \quad t_i = t_{i-1} + h_t, \quad i = 2, \dots, L-4, \quad (54)$$

where L depends on M and on the version of the procedure, ω_1 and ω_2 are suitable coefficients introduced for improving the stability of the method and $h_t = \pi/(2L + 2\omega_1 + 2\omega_2 - 5)$.

If we let $\{t_i\}_{i=-3}^L$ with $t_{-i} = \pi/2 - ih_t$ and $t_{L-3+i} = \pi + ih_t$ for $i = 1, 2, 3$, then in the sequel, we will denote with $\tilde{\phi}_j(x)$ the B-spline function of order four with support $[t_{j-4}, t_j]$ normalized to have L^2 -norm equal to one.

In the case of version \mathbf{V}_1 , we simply set $L = M$ and $\phi_j(x) = \tilde{\phi}_j(x)$ for each $j = 1, 2, \dots, M$.

Concerning version \mathbf{V}_2 , instead, we set $L = M + 1$ due to the constraint on the coordinate functions of having zero value at $x = \pi/2$. This implies that actually we consider a subspace of size M of the function space of cubic spline functions with respect to Δ . We observe that the associated B-spline functions of order four verify

$$\tilde{\phi}_j\left(\frac{\pi}{2}\right) \neq 0, \quad j = 1, 2, 3, \quad \tilde{\phi}_j\left(\frac{\pi}{2}\right) = 0, \quad j = 4, \dots, M + 1.$$

By virtue of this fact, the basis functions are chosen as follows

$$\begin{aligned} \phi_j(x) &= \frac{\tilde{\phi}_{j+1}(x) - \chi_j \tilde{\phi}_1(x)}{\|\tilde{\phi}_{j+1}(\cdot) - \chi_j \tilde{\phi}_1(\cdot)\|_2}, & \chi_j &= \frac{\tilde{\phi}_{j+1}(\pi/2)}{\tilde{\phi}_1(\pi/2)}, & j &= 1, 2, \\ \phi_j(x) &= \tilde{\phi}_{j+1}(x), & j &= 3, \dots, M. \end{aligned}$$

The used criterion for the choice of the coefficients ω_2 in (53)-(54) has been that of setting $\omega_2 = 2$ or $\omega_2 = 3$ in the case of BC $y'(\pi) = 0$ or $y(\pi) = 0$, respectively. Concerning the coefficient ω_1 the selected value depends on the version of the procedure. In particular, we set $\omega_1 = 2$ for version \mathbf{V}_1 and $\omega_1 = 1$ for the other one. In this latter case, in fact, the support of the first basis function turns out to be sufficiently large even with $\omega_1 = 1$ since constituted by two subintervals of Δ instead of only one, see Remark 2. In Tables 4-5, the obtained conditioning of the limit Jacobian $J(0, \mathbf{0})$ have been reported for problems subject to natural BCs. As one can see, for both versions of the procedure, the asymptotic behaviour of $\kappa(J(0, \mathbf{0}))$ is linear for all BCs with the exception of the problem with Dirichlet BCs at both ends for which it behaves as $O(M^{1/2})$.

It is worth mentioning that we have tested other values for the couple (ω_1, ω_2) but, among them, the best results are those here reported.

5. Numerical results

In this section we report the results of some numerical experiments we have conducted with the described procedures for the two-spectra and the half inverse problems. The reference eigenvalues used have been computed by using the MATSLISE software package [31]. The direct problems involved in the procedure have been solved by applying the BVMs described in Section 2 defined over a nonuniform mesh constituted by $N = 6M$ meshpoints with a geometric progression distribution of them near the ends of $[0, \pi]$ (see Remark 1). Concerning the vector of asymptotic corrections (26), whose entries

Table 4: Conditioning of the limit Jacobian $J(0, \mathbf{0})$ for the spline function spaces for the version \mathbf{V}_1 of the procedure.

M	$\kappa(J(0, \mathbf{0}))$	Rate	$\kappa(J(0, \mathbf{0}))$	Rate
DD BCs - $(\omega_1, \omega_2) = (2, 3)$			NN BCs - $(\omega_1, \omega_2) = (2, 2)$	
10	$6.59 + 01$	—	$5.74 + 01$	—
20	$9.92 + 01$	—	$1.03 + 02$	—
40	$1.45 + 02$	0.45	$1.92 + 02$	0.97
80	$2.08 + 02$	0.47	$3.70 + 02$	0.99
160	$2.96 + 02$	0.49	$7.24 + 02$	1.00
DN BCs - $(\omega_1, \omega_2) = (2, 2)$			ND BCs - $(\omega_1, \omega_2) = (2, 3)$	
10	$7.77 + 01$	—	$1.86 + 02$	—
20	$1.42 + 02$	—	$3.32 + 02$	—
40	$2.73 + 02$	1.03	$6.43 + 02$	1.09
80	$5.34 + 02$	1.00	$1.27 + 03$	1.02
160	$1.06 + 03$	1.00	$2.53 + 03$	1.00

are given in (9), we had to compute only the numerical eigenvalues $\lambda_k^{(h)}(0, a, b)$ due to the fact that we have considered inverse SLP subject to natural BCs for which $\lambda_k(0, a, b)$ are known in closed form. The modified Newton iterations (30) or (40) have been stopped as soon as $\|\mathbf{c}_{r+1}^{(h)} - \mathbf{c}_r^{(h)}\| < 10^{-9}$.

EXAMPLE 1. The unknown potential to be recovered is $q(x) = (e^x - x^2)/12$ starting from the knowledge of the first M eigenvalues of the two spectra of the corresponding SLPs with DD and DN BCs, respectively. We have used the function space of cubic spline functions described in Section 3.2 with $(\omega_1, \omega_2) = (3, 2)$.

In Figure 1, the errors in the reconstructed potential for $M = 5, 10$ and the BVMs with $\nu = 1$, i.e. Numerov's method, and $\nu = 3$ have been reported together with the error in the pointwise approximation provided by the Nu-

Table 5: Conditioning of the limit Jacobian $J(0, \mathbf{0})$ for the spline function spaces for the version \mathbf{V}_2 of the procedure.

M	$\kappa(J(0, \mathbf{0}))$	Rate	$\kappa(J(0, \mathbf{0}))$	Rate
DD BCs - $(\omega_1, \omega_2) = (1, 3)$			NN BCs - $(\omega_1, \omega_2) = (1, 2)$	
10	$6.46 + 01$	—	$5.71 + 01$	—
20	$9.81 + 01$	—	$1.02 + 02$	—
40	$1.44 + 02$	0.45	$1.92 + 02$	0.98
80	$2.07 + 02$	0.47	$3.69 + 02$	0.99
160	$2.96 + 02$	0.48	$7.23 + 02$	1.00
DN BCs - $(\omega_1, \omega_2) = (1, 2)$			ND BCs - $(\omega_1, \omega_2) = (1, 3)$	
10	$5.05 + 01$	—	$2.49 + 02$	—
20	$8.28 + 01$	—	$3.88 + 02$	—
40	$1.48 + 02$	1.02	$7.26 + 02$	1.29
80	$2.83 + 02$	1.03	$1.43 + 03$	1.06
160	$5.55 + 02$	1.02	$2.86 + 03$	1.01

merov method used as described in [7, Algorithm 2]. As one can see, the approach considered in this paper of looking for a continuous approximation of the potential allows to get a definitely more accurate solution (this is observed also if the comparison is done with respect to the cubic spline interpolating the grid points provided by the method in [7]). Moreover, the higher the order of the BVM the smaller the error is. On the other hand, we must mention the fact that, for a given M , the computational effort increases with respect to ν due to the larger bandwidth of the matrices involved. Nevertheless, this is only a minor disadvantage because (as emphasized in [8]) in applications it is nearly always the scarcity of available data, rather than computing resources, that limits available accuracy.

EXAMPLE 2. In this second example, we have used the trigonometric func-

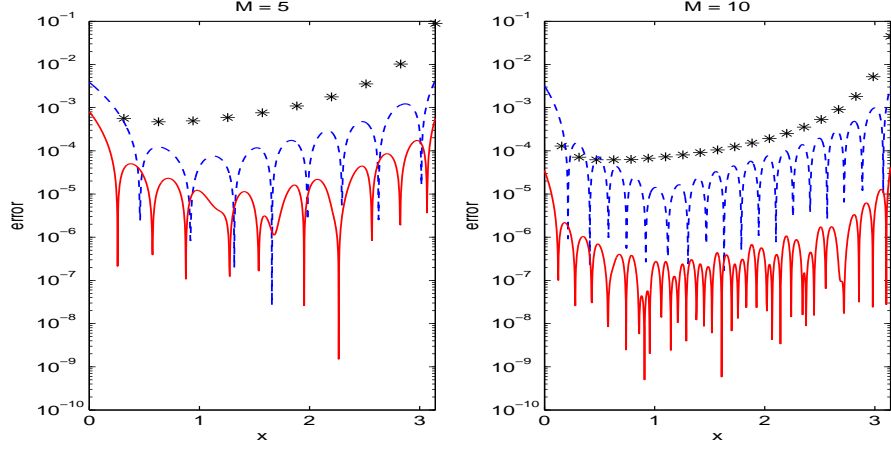


Figure 1: Error in the reconstruction of $q(x) = (e^x - x^2)/12$ by using the spline functions and the BVMs with $\nu = 1$ (dashed line) and $\nu = 3$ (solid line) compared with the pointwise approximation provided by the Numerov method [7].

tion space spanned by the basis functions in (34) to recover the discontinuous potential

$$q(x) = \begin{cases} 0 & 0 \leq x < \pi/10 \\ 7x/\pi - 0.7 & \pi/10 \leq x < 3\pi/10 \\ 3.5 - 7x/\pi & 3\pi/10 \leq x < \pi/2 \\ 0 & \pi/2 \leq x < 7\pi/10 \\ 4 & 7\pi/10 \leq x < 9\pi/10 \\ 2 & 9\pi/10 \leq x \leq \pi \end{cases} \quad (55)$$

starting from the knowledge of the corresponding NN-ND spectra. In the first three subplots of Figure 2, together with the exact potential, the approximations obtained by using the BVM of order 8 are displayed for $M = 10, 20, 30$ couples of known eigenvalues. In addition, in the last subplot we have reported the norms $\|q - \phi(\cdot, \mathbf{c}^*)\|_2$ (dashed line) and $\|\phi(\cdot, \mathbf{c}^*) - \phi(\cdot, \mathbf{c})\|_2$ (solid line) versus M where, we recall, $\phi(\cdot, \mathbf{c}^*)$ denotes the best approximation in L^2 -norm of q over the considered function space while $\phi(\cdot, \mathbf{c})$ is the approximation computed by solving the inverse problem. From the curves in the last subplot one deduces that $\|\phi(\cdot, \mathbf{c}) - \phi(\cdot, \mathbf{c}^*)\|_2 \ll \|q - \phi(\cdot, \mathbf{c}^*)\|_2$ and, consequently,

$$\|q - \phi(\cdot, \mathbf{c}^*)\|_2 \leq \|q - \phi(\cdot, \mathbf{c})\|_2 \leq \|q - \phi(\cdot, \mathbf{c}^*)\|_2 + \|\phi(\cdot, \mathbf{c}^*) - \phi(\cdot, \mathbf{c})\|_2$$

$$\approx \|q - \phi(\cdot, \mathbf{c}^*)\|_2.$$

The error in the approximation computed is therefore very close to the minimum error for the used function space and this is a surely satisfactory result.

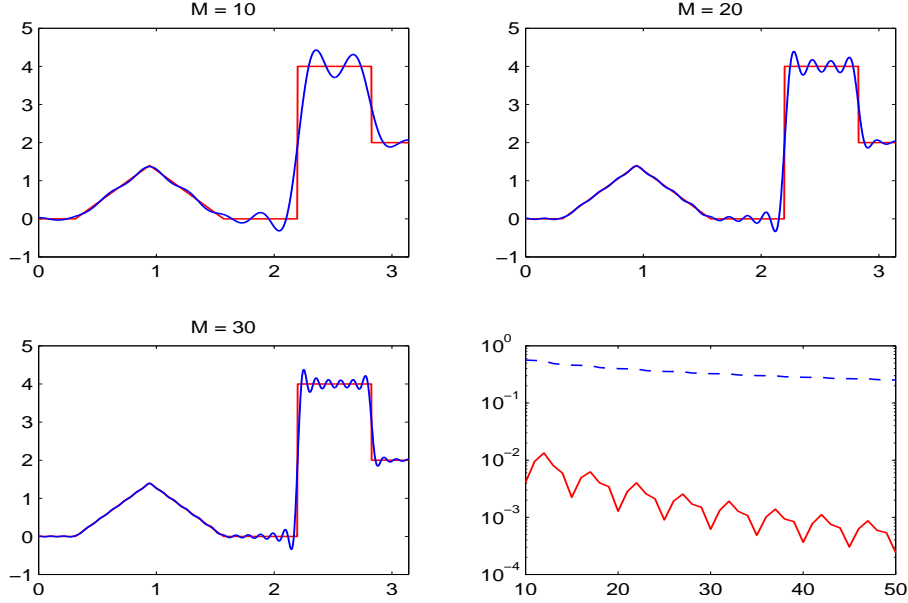


Figure 2: Reconstruction of the discontinuous potential (55) with trigonometric polynomials and corresponding error in the approximation.

EXAMPLE 3. This is an example for the half inverse problem. The potential to be recovered over $(\pi/2, \pi]$ is

$$q(x) = \frac{1}{2}x^2(\pi - x). \quad (56)$$

In order to reconstruct it, we have applied the two versions of the procedure for solving the corresponding inverse problems associated to the four possible couples of natural BCs. In each case, we have used the first $M = 10$ eigenvalues of the spectrum, the function space of trigonometric polynomials described in Section 4.1 and the BVM of order $p = 8$. The errors in the so-obtained approximations have been reported in Figure 3. Clearly, by construction, the version \mathbf{V}_2 of the procedure provides more accurate results

near $x = \pi/2$. Moreover, this higher accuracy holds over almost the entire interval $[\pi/2, \pi]$ in the case where the BC at the right end is $y(\pi) = 0$.

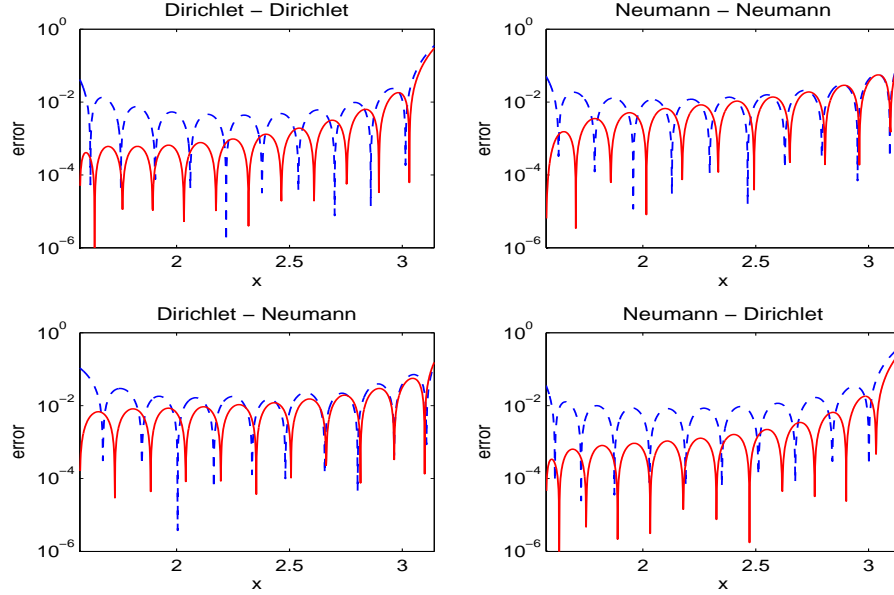


Figure 3: Error in the reconstruction of the partially known potential (56) by using version \mathbf{V}_1 (dashed line) and version \mathbf{V}_2 (solid line) of the procedure with trigonometric polynomials.

EXAMPLE 4. In this last example, the unknown potential is the non-smooth continuous function

$$q(x) = |3 - |x^2 - 3|| \quad (57)$$

which must be reconstructed over $(\pi/2, \pi]$ from the knowledge of the eigenvalues of the corresponding SLP with BCs $y'(0) = y(\pi) = 0$. We have applied the version \mathbf{V}_2 with cubic spline functions and the BVM of order $p = 8$. The results obtained for $M = 5, 10$ and $M = 20$ known eigenvalues have been reported in Figure 4. We observe that even though the exact solution is only continuous the method provides a satisfactory approximation and the accuracy improves as M increases.

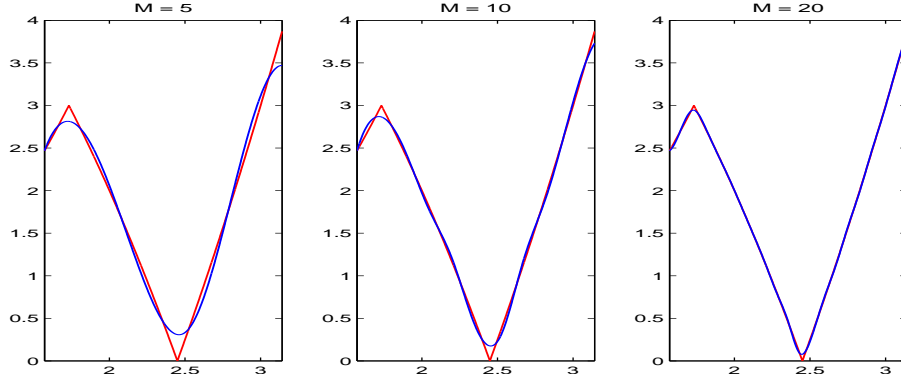


Figure 4: Reconstruction of the partially known potential (57) by applying version \mathbf{V}_2 of the method with cubic spline functions.

6. Conclusions

The numerical procedures proposed for the solution of the two-spectra and the half inverse SLPs have provided very positive results which, for the former problem, are competitive with respect to those given by the method presented in [7]. The modified Newton method used for solving the system of nonlinear equations involved in the procedures turns out to have good convergence properties in the case where the potential to be recovered is sufficiently close to a constant function. With the aim of relaxing this constraint, an interesting topic for future investigation could be the development of alternative procedures, based on optimization techniques like the Gauss-Newton or trust-region methods, for the solution of such systems of nonlinear equations.

References

- [1] G. Borg, Eine Umkehrung der Sturm-Liouvilleschen Eigenwertaufgabe, Acta Math. 78 (1946) 732-753.
- [2] H. Hochstad, B. Lieberman, An inverse Sturm-Liouville problem with mixed given data, SIAM J. Appl. Math. 34 (1978) 676-680.
- [3] V.A. Marchenko, Sturm-Liouville Operators and Applications, Basel, Birkhäuser, 1986.

- [4] J. Pöschel, E. Trubowitz, *Inverse Spectral Theory*, London, Academic Press, 1987.
- [5] M. Marletta, R. Weikard, Weak stability for an inverse Sturm-Liouville problem with finite spectral data and complex potential, *Inverse Problems* 21 (2005) 1275-1290.
- [6] A.L. Andrew, Numerov's method for inverse Sturm-Liouville problems, *Inverse Problems* 21 (2005) 223-238.
- [7] A.L. Andrew, Computing Sturm-Liouville potentials from two spectra, *Inverse Problems* 22 (2006) 2069-2081.
- [8] A.L. Andrew, Finite difference methods for half inverse Sturm-Liouville problems, *Appl. Math. Comput.* 218 (2011) 445-457.
- [9] C. Böckmann, A. Kammanee, Broyden method for inverse non-symmetric Sturm-Liouville problems, *BIT* 51 (2011) 513-528.
- [10] R.H. Fabiano, R. Knobel, B.D. Lowe, A finite-difference algorithm for an inverse Sturm-Liouville problem, *IMA J. Numer. Anal.* 15 (1995) 75-88.
- [11] G.M.L. Gladwell, *Inverse Problems in Vibration* 2nd edn, Dordrecht: Kluwer Academic Publishers, 2004.
- [12] O.H. Hald, The inverse Sturm-Liouville problem and the Rayleigh-Ritz method, *Math. Comp.* 32 (1978) 687-705.
- [13] M. Ignatiev, V. Yurko, Numerical methods for solving inverse Sturm-Liouville problems, *Result. Math.* 52 (2008) 63-74.
- [14] A. Kammanee, C. Böckmann, Determination of partially known Sturm-Liouville potentials, *Appl. Math. Comp.* 204 (2008) 928-937.
- [15] A. Kammanee, C. Böckmann, Boundary value method for inverse Sturm-Liouville problems, *Appl. Math. Comp.* 214 (2009) 342-352.
- [16] M. Neher, Enclosing solutions of an inverse Sturm-Liouville problem with finite data, *Computing* 53 (1994) 379-395.

- [17] M. Raffler, C. Böckmann, Reconstructive method for inverse Sturm-Liouville problems with discontinuous potentials, *Inverse Problems* 23 (2007) 933-946.
- [18] N. Röhl, A least-squares functional for solving inverse Sturm-Liouville problems, *Inverse Problems* 21 (2005) 2009-2017.
- [19] W. Rundell, P.E. Sacks, Reconstruction techniques for classical Sturm-Liouville problems, *Math. Comp.* 58 (1992) 161-183.
- [20] V.V. Ternovskii, M.M. Khapaev, Reconstruction of potentials in the Sturm-Liouville inverse problem by the variational method, *Dokl. Math.* 73 (2006) 107-111.
- [21] R.S. Anderssen, F.R. de Hoog, On the correction of finite difference eigenvalue approximations for Sturm-Liouville problems with general boundary conditions, *BIT* 24 (1984) 401-412.
- [22] J.W. Paine, F.R. de Hoog, R.S. Anderseen, On the correction of finite difference eigenvalue approximations for Sturm-Liouville problems, *Computing* 26 (1981) 123-139.
- [23] A.L. Andrew, Asymptotic correction of Numerov's eigenvalue estimates with natural boundary conditions, *J. Comput. Appl. Math.* 125 (2000) 359-366.
- [24] A.L. Andrew, Asymptotic correction of Numerov's eigenvalue estimates with general boundary conditions, *ANZIAM J.* 44 (2002) C1-C19.
- [25] A.L. Andrew, J.W. Paine, Correction of Numerov's eigenvalue estimates, *Numer. Math.* 47 (1985) 289-300.
- [26] L. Aceto, P. Ghelardoni, C. Magherini, Boundary Value Methods as an extension of Numerov's method for Sturm-Liouville eigenvalue estimates, *Appl. Numer. Math.* 59 (2009) 1644-1656.
- [27] L. Aceto, P. Ghelardoni, C. Magherini, BVMs for Sturm-Liouville eigenvalue estimates with general boundary conditions, *JNAIAM* 4 (2009) 113-127.
- [28] P. Ghelardoni, Approximations of Sturm-Liouville eigenvalues using Boundary Value Methods, *Appl. Numer. Math.* 23 (1997) 311-325.

- [29] P. Ghelardoni, C. Magherini, BVMS for computing Sturm-Liouville symmetric potentials, *Appl. Math. Comput.* 217 (2010) 3032-3045.
- [30] L. Brugnano, D. Trigiante, *Solving ODEs by Linear Multistep Initial and Boundary Value Methods*, Amsterdam, Gordon & Breach, 1998.
- [31] V. Ledoux, M. Van Daele, G. Vanden Berghe, Matslise: A Matlab package for the Numerical Solution of Sturm-Liouville and Schrödinger equations, *ACM Trans. Math. Software* 31 (2005) 532-554. Available at <http://users.ugent.be/~vledoux/MATSLISE/>